

# **Drug Repurposing for COVID-19 using Graph Neural Network with Genetic, Mechanistic, and Epidemiological Validation**

**Authors:** Kanglin Hsieh, Ph.D.,<sup>1</sup> Yinyin Wang, M.S.,<sup>2</sup> Luyao Chen, M.S.,<sup>1</sup> Zhongming Zhao, Ph.D.,<sup>3</sup> Sean Savitz, M.D.,<sup>4</sup> Xiaoqian Jiang, Ph.D.,<sup>1</sup> Jing Tang, Ph.D.,<sup>2</sup> Yejin Kim, Ph.D.<sup>1\*</sup>

## **Supplementary Information Index**

Supplementary Notes 1: Transfer learning

Supplementary Notes 2: Calculating the treatment effect

Supplementary Notes 3: Re-ordering the validated drugs

Supplementary Notes 4: Genetic validation using gene set enrichment analysis

Supplementary Table S1: Link prediction accuracy in the SARS-CoV-2 knowledge graph.

Supplementary Table S2: ATT score of 138 drugs that were in EHRs and initial 3,635 drugs.

Supplementary Table S3: Full list of repurposable drugs

Supplementary Table S4: Full list of drug combinations from the top drugs.

Supplementary Figure S1: The SARS-CoV-2 Knowledge Graph

Supplementary Figure S2: Interactive t-sne plot

Supplementary Figure S3: External validation (a) Accuracy was measured in the intersection of candidate drugs and external validation sources. (b) Cohort selection and propensity score matching in EHRs.